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Predictors of the stability of high entropy alloys: is the entropy of mixing sufficient?[1] M. CLAUDIA TROPAREVSKY, JAMES R. MORRIS, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, PAUL KENT, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, G. MALCOLM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA — High entropy alloys (HEAs) have attracted extensive attention due to their remarkable combination of strength, ductility, thermal stability, corrosion and wear resistance. However, little is known about why these alloys are stable in a single-phase solid solution or how to predict which combinations of elements will form a single phase HEA. Here, we present density functional theory calculations of the heat of formation of several HEAs in an effort to assess the role of the entropy of mixing in the stability of these alloys. The systems studied here include both single-phase and multi-phase alloys. The heats of formation show no significant differences, regardless of their single or multi phase formation, and no trends that could explain the stability of the single phase materials. Moreover, all of the calculated heats of formation are positive. These findings indicate that the entropy of mixing is insufficient to explain the unique stability of these alloys, and highlights the need for new criteria to explain the formation of single-phase solid solutions. We also discuss the minimum energy structures of several FCC and BCC alloys as well as their relative phase stability.

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